

Table S2. The binding free energy for 1b/Erastin-SLC7A11 (kcal/mol)

system	Polar contributions		Non-polar contributions		ΔG_{bind}
	ΔG_{ele}	$\Delta G_{\text{ele,sol}}$	ΔG_{vdw}	$\Delta G_{\text{nonpol,sol}}$	
1b-SLC7A11	-23.778	36.686	-46.129	-5.616	-38.837
Erastin-SLC7A11	-3.149	18.752	-39.117	-4.900	-28.414